

* * * * * Welcome to STN International * * * * *

NEWS 1 Web Page for STN Seminar Schedule - N. America
NEWS 2 DEC 01 ChemPort single article sales feature unavailable
NEWS 3 JUN 01 CAS REGISTRY Source of Registration (SR) searching
enhanced on STN
NEWS 4 JUN 26 NUTRACEUT and PHARMAML no longer updated
NEWS 5 JUN 29 IMSCOPROFILE now reloaded monthly
NEWS 6 JUN 29 EPFULL adds Simultaneous Left and Right Truncation
(SLART) to AB, MCLM, and TI fields
NEWS 7 JUL 09 PATDPAFULL adds Simultaneous Left and Right
Truncation (SLART) to AB, CLM, MCLM, and TI fields
NEWS 8 JUL 14 USGENE enhances coverage of patent sequence location
(PSL) data
NEWS 9 JUL 27 CA/CAPLUS enhanced with new citing references
NEWS 10 JUL 16 GBFULL adds patent backfile data to 1855
NEWS 11 JUL 21 USGENE adds bibliographic and sequence information
NEWS 12 JUL 28 EPFULL adds first-page images and applicant-cited
references
NEWS 13 JUL 28 INPADOCDB and INPAFAMDB add Russian legal status data
NEWS 14 AUG 08 Improve STN by completing a survey and be entered to
win a gift card
NEWS 15 AUG 10 Time limit for inactive STN sessions doubles to 40
minutes

NEWS EXPRESS MAY 26 09 CURRENT WINDOWS VERSION IS V8.4,
AND CURRENT DISCOVER FILE IS DATED 06 APRIL 2009.

NEWS HOURS STN Operating Hours Plus Help Desk Availability
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Enter NEWS followed by the item number or name to see news on that
specific topic.

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* *
* Please take a couple of minutes to complete our short survey. Your *
* name will be entered to win one of five \$20 Amazon.com gift cards. *
* *
* See NEWS 14 for details or go directly to the survey at: *
* <http://www.zoomerang.com/Survey/?p=WEB229H4S8Q5UL> *
* *

* * * * * STN Columbus * * * * *

FILE 'HOME' ENTERED AT 11:51:54 ON 10 AUG 2009

=>

Uploading

THIS COMMAND NOT AVAILABLE IN THE CURRENT FILE

Do you want to switch to the Registry File?

Choice (Y/n):

Switching to the Registry File...

Some commands only work in certain files. For example, the EXPAND
command can only be used to look at the index in a file which has an

index. Enter "HELP COMMANDS" at an arrow prompt (=>) for a list of commands which can be used in this file.

=> FILE REGISTRY

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	0.22	0.22

FILE 'REGISTRY' ENTERED AT 11:52:19 ON 10 AUG 2009
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Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 9 AUG 2009 HIGHEST RN 1173690-68-0
DICTIONARY FILE UPDATES: 9 AUG 2009 HIGHEST RN 1173690-68-0

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH January 9, 2009.

Please note that search-term pricing does apply when conducting SmartSELECT searches.

REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of experimental property data in the original document. For information on property searching in REGISTRY, refer to:

<http://www.cas.org/support/stngen/stndoc/properties.html>

=>

Uploading C:\Program Files\Stnexp\Queries\10594231-cyclic.str

L1 STRUCTURE UPLOADED

=> d 11

L1 HAS NO ANSWERS

L1 STR

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

Structure attributes must be viewed using STN Express query preparation.

=>

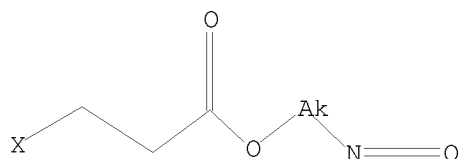
Uploading C:\Program Files\Stnexp\Queries\10594231-alkyl.str

L2 STRUCTURE UPLOADED

=> d 12

L2 HAS NO ANSWERS

L2 STR



Structure attributes must be viewed using STN Express query preparation.

```
=> d 11
L1 HAS NO ANSWERS
L1          STR
*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***
```

Structure attributes must be viewed using STN Express query preparation.

```
=>
Uploading C:\Program Files\Stnexp\Queries\10594231-cyclic.str
```

```
L3          STRUCTURE UPLOADED
```

```
=> d 13
L3 HAS NO ANSWERS
L3          STR
*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***
```

Structure attributes must be viewed using STN Express query preparation.

```
=> s 11
SAMPLE SEARCH INITIATED 11:53:30 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED -      20560 TO ITERATE

  9.7% PROCESSED      2000 ITERATIONS                      0 ANSWERS
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS:  ONLINE  **COMPLETE**
                        BATCH   **COMPLETE**
PROJECTED ITERATIONS:   402613 TO   419787
PROJECTED ANSWERS:      0 TO      0
```

```
L4          0 SEA SSS SAM L1
```

```
=> s 11 full
FULL SEARCH INITIATED 11:53:35 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED -   406408 TO ITERATE
```

```
 77.2% PROCESSED   313548 ITERATIONS                      21 ANSWERS

 94.0% PROCESSED   381859 ITERATIONS                      21 ANSWERS

100.0% PROCESSED   406408 ITERATIONS                      21 ANSWERS
SEARCH TIME: 00.00.33
```

```
L5          21 SEA SSS FUL L1
```

```
=> s 12
SAMPLE SEARCH INITIATED 11:54:15 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED -      20561 TO ITERATE
```

```
  9.7% PROCESSED      2000 ITERATIONS                      3 ANSWERS
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS:  ONLINE  **COMPLETE**
                        BATCH   **COMPLETE**
```

PROJECTED ITERATIONS: 402633 TO 419807
PROJECTED ANSWERS: 283 TO 949

L6 3 SEA SSS SAM L2

=> s l2 full
FULL SEARCH INITIATED 11:54:19 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 406458 TO ITERATE

74.7% PROCESSED	303779 ITERATIONS	501 ANSWERS
93.7% PROCESSED	381049 ITERATIONS	501 ANSWERS
100.0% PROCESSED	406458 ITERATIONS	501 ANSWERS

SEARCH TIME: 00.00.34

L7 501 SEA SSS FUL L2

=> file caplus		
COST IN U.S. DOLLARS	SINCE FILE	TOTAL
	ENTRY	SESSION
FULL ESTIMATED COST	373.20	373.42

FILE 'CAPLUS' ENTERED AT 11:55:02 ON 10 AUG 2009
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FILE COVERS 1907 - 10 Aug 2009 VOL 151 ISS 7
FILE LAST UPDATED: 9 Aug 2009 (20090809/ED)
REVISED CLASS FIELDS (/NCL) LAST RELOADED: Jun 2009
USPTO MANUAL OF CLASSIFICATIONS THESAURUS ISSUE DATE: Jun 2009

CAPLUS now includes complete International Patent Classification (IPC) reclassification data for the second quarter of 2009.

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This file contains CAS Registry Numbers for easy and accurate substance identification.

The ALL, BIB, MAX, and STD display formats in the CA/CAPLUS family of databases have been updated to include new citing references information. This enhancement may impact record import into database management software. For additional information, refer to NEWS 9.

=> s l5
L8 8 L5

```

=> s 17
L9          164 L7

=> s 15 or 17
           8 L5
           164 L7
L10         172 L5 OR L7

=> s 110 not py > 2005
           5386437 PY > 2005
L11         143 L10 NOT PY > 2005

=> s 111 and triethylamine
           38935 TRIETHYLAMINE
L12         1 L11 AND TRIETHYLAMINE

=> s 111 and trialkylamine
           1182 TRIALKYLAMINE
L13         0 L11 AND TRIALKYLAMINE

=> s 111 and trimethylamine
           16342 TRIMETHYLAMINE
L14         0 L11 AND TRIMETHYLAMINE

=> s 11 and amine
    REGISTRY INITIATED
Substance data SEARCH and crossover from CAS REGISTRY in progress...
Use DISPLAY HITSTR (or FHITSTR) to directly view retrieved structures.

```

```

SAMPLE SEARCH INITIATED 11:56:12 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 20560 TO ITERATE

```

```

    9.7% PROCESSED      2000 ITERATIONS                      0 ANSWERS
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
SEARCH TIME: 00.00.01

```

```

FULL FILE PROJECTIONS:  ONLINE  **COMPLETE**
                        BATCH   **COMPLETE**
PROJECTED ITERATIONS:   402613 TO 419787
PROJECTED ANSWERS:      0 TO      0

```

```

L15          0 SEA SSS SAM L1

```

```

L16          0 L15

```

```

           308463 AMINE
L17         0 L16 AND AMINE

```

```

=> file caplus
COST IN U.S. DOLLARS          SINCE FILE      TOTAL
                                ENTRY          SESSION
FULL ESTIMATED COST          2.74          386.60

```

```

FILE 'CAPLUS' ENTERED AT 11:56:19 ON 10 AUG 2009
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```

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This file contains CAS Registry Numbers for easy and accurate substance identification.

The ALL, BIB, MAX, and STD display formats in the CA/CAPLUS family of databases have been updated to include new citing references information. This enhancement may impact record import into database management software. For additional information, refer to NEWS 9.

```
=> s l11 and amine
      308463 AMINE
L18      10 L11 AND AMINE

=> s l18 or l12
L19      10 L18 OR L12

=> s l11 and acrylate
      212923 ACRYLATE
L20      5 L11 AND ACRYLATE

=> s l11 and methacrylate
      246682 METHACRYLATE
L21      5 L11 AND METHACRYLATE

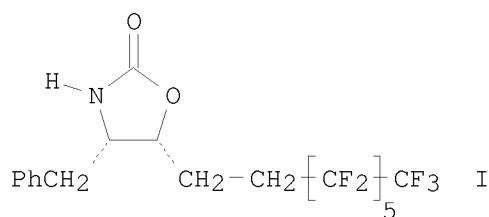
=> s l21 or l20
L22      8 L21 OR L20

=> s l22 and l19
L23      0 L22 AND L19
```

```
=> d l19 ibib abs hitstr 1-
YOU HAVE REQUESTED DATA FROM 10 ANSWERS - CONTINUE? Y/(N):y
```

```
L19 ANSWER 1 OF 10 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 2005:1126962 CAPLUS
DOCUMENT NUMBER: 144:51485
TITLE: Practical synthesis of fluorous oxazolidinone chiral
auxiliaries from  $\alpha$ -amino acids
```

AUTHOR(S): Hein, Jason E.; Geary, Laina M.; Jaworski, Ashley A.;
Hultin, Philip G.
CORPORATE SOURCE: Department of Chemistry, University of Manitoba,
Winnipeg, MB, R3T 2N2, Can.
SOURCE: Journal of Organic Chemistry (2005), 70(24), 9940-9946
CODEN: JOCEAH; ISSN: 0022-3263
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 144:51485
GI



AB A series of fluorous-supported oxazolidinone chiral auxiliaries, e.g., I, has been prepared using a versatile and general five-step pathway, starting from readily available chiral α -amino acids. The key feature of this synthesis was the efficient generation of a suitably active perfluoroalkyllithium species. By use of this protocol, the auxiliaries can be obtained in high enantiomeric purity and on multigram scales from L-phenylalanine and L-valine with good overall yields. The methodol. also incorporated fluorous solid-phase extraction on the large scale, allowing bulk quantities of fluorous compds. to be purified from the crude reaction mixture

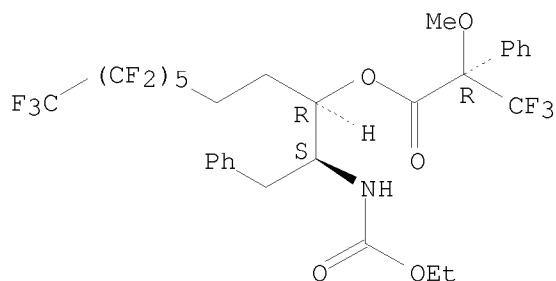
IT 871210-28-5P 871210-29-6P 871210-30-9P
871210-31-0P 871210-32-1P 871210-33-2P
871210-34-3P 871210-35-4P

RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of fluorous esters via esterification of fluorous N-carbamoyl amino alcs. with MTPA)

RN 871210-28-5 CAPLUS

CN Benzeneacetic acid, α -methoxy- α -(trifluoromethyl)-,
(1R)-1-[(1S)-1-[(ethoxycarbonyl)amino]-2-phenylethyl]-
4,4,5,5,6,6,7,7,8,8,9,9,9-tridecafluorononyl ester, (α R)- (CA INDEX
NAME)

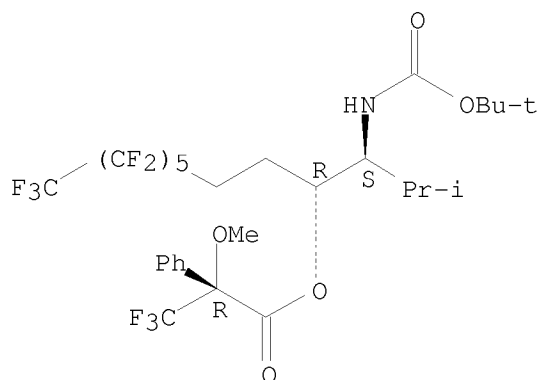
Absolute stereochemistry. Rotation (-).



RN 871210-29-6 CAPLUS

CN Benzeneacetic acid, α -methoxy- α -(trifluoromethyl)-,
 (1R)-1-[(1S)-1-[[(1,1-dimethylethoxy)carbonyl]amino]-2-methylpropyl]-
 4,4,5,5,6,6,7,7,8,8,9,9,9-tridecafluorononyl ester, (α R)- (CA INDEX
 NAME)

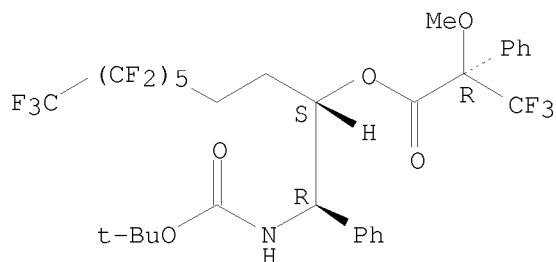
Absolute stereochemistry. Rotation (+).



RN 871210-30-9 CAPLUS

CN Benzeneacetic acid, α -methoxy- α -(trifluoromethyl)-,
 (1S)-1-[(R)-[[(1,1-dimethylethoxy)carbonyl]amino]phenylmethyl]-
 4,4,5,5,6,6,7,7,8,8,9,9,9-tridecafluorononyl ester, (α R)- (CA INDEX
 NAME)

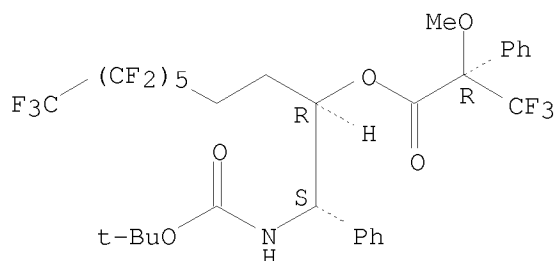
Absolute stereochemistry.



RN 871210-31-0 CAPLUS

CN Benzeneacetic acid, α -methoxy- α -(trifluoromethyl)-,
 (1R)-1-[(S)-[[(1,1-dimethylethoxy)carbonyl]amino]phenylmethyl]-
 4,4,5,5,6,6,7,7,8,8,9,9,9-tridecafluorononyl ester, (α R)- (CA INDEX
 NAME)

Absolute stereochemistry.

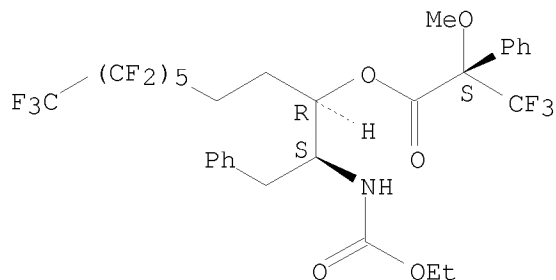


RN 871210-32-1 CAPLUS

CN Benzeneacetic acid, α -methoxy- α -(trifluoromethyl)-,
 (1R)-1-[(1S)-1-[(ethoxycarbonyl)amino]-2-phenylethyl]-

4,4,5,5,6,6,7,7,8,8,9,9,9-tridecafluorononyl ester, (α S)- (CA INDEX NAME)

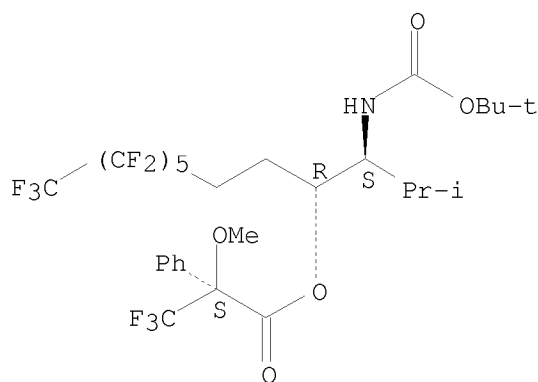
Absolute stereochemistry. Rotation (+).



RN 871210-33-2 CAPLUS

CN Benzeneacetic acid, α -methoxy- α -(trifluoromethyl)-, (1R)-1-[(1S)-1-[[[(1,1-dimethylethoxy)carbonyl]amino]-2-methylpropyl]-4,4,5,5,6,6,7,7,8,8,9,9,9-tridecafluorononyl ester, (α S)- (CA INDEX NAME)

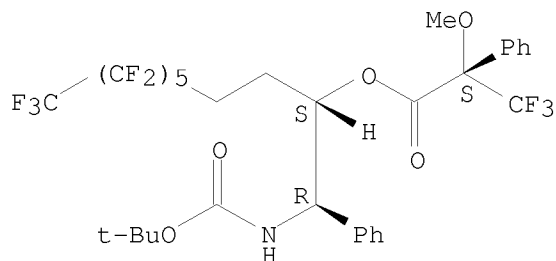
Absolute stereochemistry. Rotation (+).



RN 871210-34-3 CAPLUS

CN Benzeneacetic acid, α -methoxy- α -(trifluoromethyl)-, (1S)-1-[(R)-[[[(1,1-dimethylethoxy)carbonyl]amino]phenylmethyl]-4,4,5,5,6,6,7,7,8,8,9,9,9-tridecafluorononyl ester, (α S)- (CA INDEX NAME)

Absolute stereochemistry.

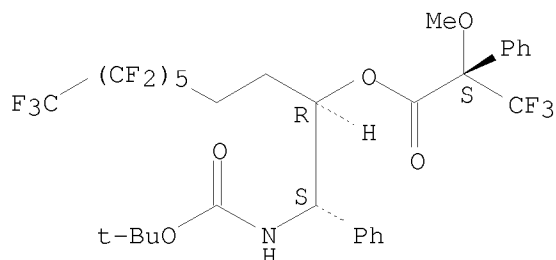


RN 871210-35-4 CAPLUS

CN Benzeneacetic acid, α -methoxy- α -(trifluoromethyl)-, (1R)-1-[(S)-[[[(1,1-dimethylethoxy)carbonyl]amino]phenylmethyl]-4,4,5,5,6,6,7,7,8,8,9,9,9-tridecafluorononyl ester, (α S)- (CA INDEX NAME)

NAME)

Absolute stereochemistry.



OS.CITING REF COUNT: 21 THERE ARE 21 CAPLUS RECORDS THAT CITE THIS
RECORD (22 CITINGS)
REFERENCE COUNT: 50 THERE ARE 50 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L19 ANSWER 2 OF 10 CAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 2000:665369 CAPLUS

DOCUMENT NUMBER: 133:362943

TITLE: One-pot synthesis of N-formyl-O-acyl-threo- and
erythro-DL- β -phenylserine ethyl esters and their
antiviral properties

AUTHOR(S): Straukas, Juozapas; Dirvianskyte, Nijole; Butkus,
Eugenius

CORPORATE SOURCE: Institute of Biochemistry, Vilnius, Lithuania

SOURCE: Journal fuer Praktische Chemie (Weinheim, Germany)

(2000), 342(7), 715-719

CODEN: JPCHF4; ISSN: 1436-9966

PUBLISHER: Wiley-VCH Verlag GmbH

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 133:362943

AB A series of N-formyl-O-acyl- β -phenylserine derivs. were prepared by the
interaction of N-acyl- β -phenylserine Et esters with formic acid in
presence of 1.5% HF. One-pot acyl group N \rightarrow O migration followed
N-formylation under elaborated reaction conditions. The kinetics of the
reaction were investigated. The carboxylic acid moiety in the structure
of β -phenylserine had a strong influence on the reproduction of the used
test-viruses. The toxicity and antiviral activity is dependent on the
diastereomeric forms of evaluated compds.

IT 306970-85-4P

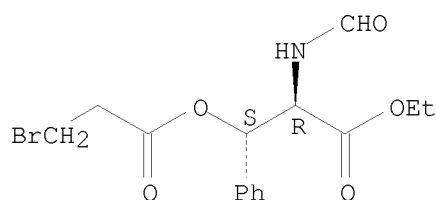
RL: BAC (Biological activity or effector, except adverse); BSU (Biological
study, unclassified); SPN (Synthetic preparation); BIOL (Biological
study); PREP (Preparation)

(synthesis of N-formyl-O-acyl-threo and erythro- β -phenylserine Et
esters and their antiviral properties and toxicities)

RN 306970-85-4 CAPLUS

CN D-Phenylalanine, β -(3-bromo-1-oxopropoxy)-N-formyl-, ethyl ester,
(β S)-rel- (CA INDEX NAME)

Relative stereochemistry.



REFERENCE COUNT: 15 THERE ARE 15 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L19 ANSWER 3 OF 10 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 2000:293396 CAPLUS
DOCUMENT NUMBER: 133:58969
TITLE: Enantioselective Total Syntheses of
13,14,15-Isocrambescidin 800 and
13,14,15-Isocrambescidin 657
AUTHOR(S): Coffey, D. Scott; Overman, Larry E.; Stappenbeck,
Frank
CORPORATE SOURCE: Department of Chemistry, University of California,
Irvine, CA, 92697-2025, USA
SOURCE: Journal of the American Chemical Society (2000),
122(20), 4904-4914
CODEN: JACSAT; ISSN: 0002-7863
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 133:58969
GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

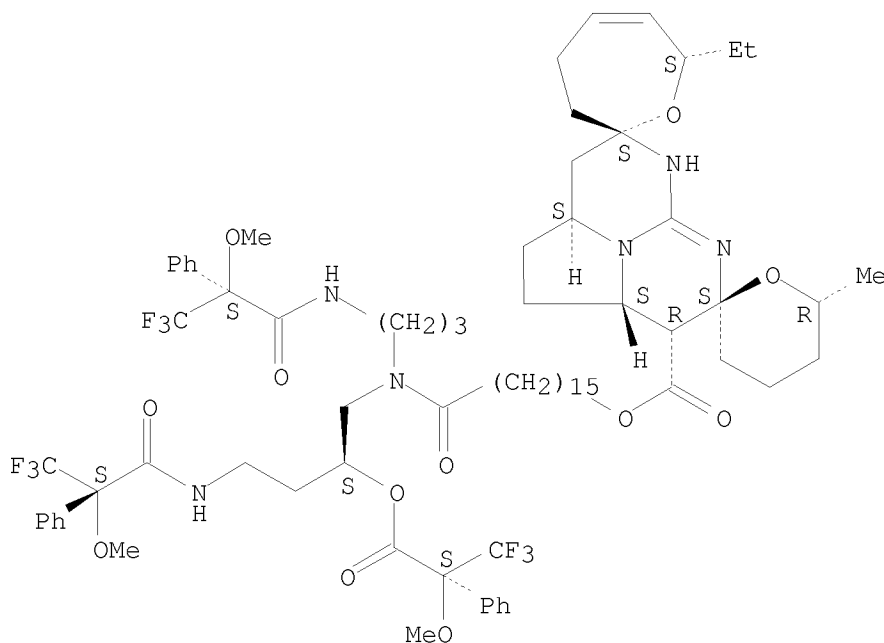
AB The first total syntheses of 13,14,15-isocrambescidin 800 [I·Cl⁻; R = NH(CH₂CH₂CH₂NH₂)CH₂CH(OH)CH₂CH₂NH₂-(S)] and 13,14,15-isocrambescidin 657 (I; R = O-) were accomplished in convergent fashion. The central strategic step was a tethered Biginelli condensation of guanidine amina I·HCl [TIPS = Si(CHMe₂)₃] and β-ketoester, (R)-H₂C:CHCH₂O₂C(CH₂)₁₅O₂CCH₂C(:O)(CH₂)₃CHMeOSiMe₂CMe₃, to give 1-iminohexahydropyrrolo[1,2-c]pyrimidine carboxylic ester III·HCl [R₁ = (CH₂)₁₅CO₂CH₂CH:CH₂, R₂ = TBDMS, R₃ = TIPS; TBDMS = SiMe₂CMe₃]. This step united all the heavy atoms of the pentacyclic guanidine nucleus and set the critical trans C10-C13 stereorelationship. Acidic treatment of derivative III·HCl [R₁ = (CH₂)₁₅CO₂CH₂CH:CH₂; R₂ = R₃ = H] triggered tricyclization to generate pentacyclic guanidine IV·Cl⁻ in high yield. After cleavage of the allyl ester, the derived acid underwent coordinated epimerization at C14 and C15 in the presence of triethylamine to form the pentacyclic isocrambescidin nucleus. The synthesis of I was achieved in 11% overall yield from amine V by a sequence involving five isolated intermediates. As detailed in the preceding account, V can be accessed from com. available 3-butyn-1-ol in 30% overall yield by way of nine isolated and purified intermediates. Mosher derivs. were prepared from (S)-(-)-α-methoxy-α-(trifluoromethyl)phenylacetic acid and natural I [R = NH(CH₂CH₂CH₂NH₂)CH₂CH(OH)CH₂CH₂NH₂-(S)], synthetic I [R = NH(CH₂CH₂CH₂NH₂)CH₂CH(OH)CH₂CH₂NH₂-(S)], and synthetic C43 epimer I·2HCl·Cl⁻ [R = NH(CH₂CH₂CH₂NH₂)CH₂CH(OH)CH₂CH₂NH₂-(R)]. Anal. by 19F NMR showed that the Mosher derivs. of natural and synthetic I [R = NH(CH₂CH₂CH₂NH₂)CH₂CH(OH)CH₂CH₂NH₂-(S)] were identical, thus establishing for the first time that the stereochem. of 13,14,15-isocrambescidin 800 [I·Cl⁻; R = NH(CH₂CH₂CH₂NH₂)CH₂CH(OH)CH₂CH₂NH₂-(S)] at C43 is S. The mechanism of the tricyclization and epimerization steps is discussed, as are the relative energies of the 13,14,15-isocrambescidin, 13,15-epicrambescidin, and 13-epicrambescidin guanidine moieties.

IT 276878-02-5P 276878-03-6P
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(enantioselective total syntheses of isocrambescidin 800 and isocrambescidin 657)

RN 276878-02-5 CAPLUS
 CN Dispiro[oxepin-2(3H),4'-[4H-5,6,8b]triazacacenaphthylene-7'(5'H),2''-[2H]pyran]-8'-carboxylic acid, 7-ethyl-1',2',2'a,3',3'',4,4'',5'',6'',7,8',8'a-dodecahydro-6''-methyl-, 16-oxo-16-[[(2S)-2-[(2S)-3,3,3-trifluoro-2-methoxy-1-oxo-2-phenylpropoxy]-4-[[(2S)-3,3,3-trifluoro-2-methoxy-1-oxo-2-phenylpropyl]amino]butyl][3-[[(2S)-3,3,3-trifluoro-2-methoxy-1-oxo-2-phenylpropyl]amino]propyl]amino]hexadecyl ester, trihydrochloride, (2S,2''S,2'aS,6''R,7S,8'R,8'aS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A

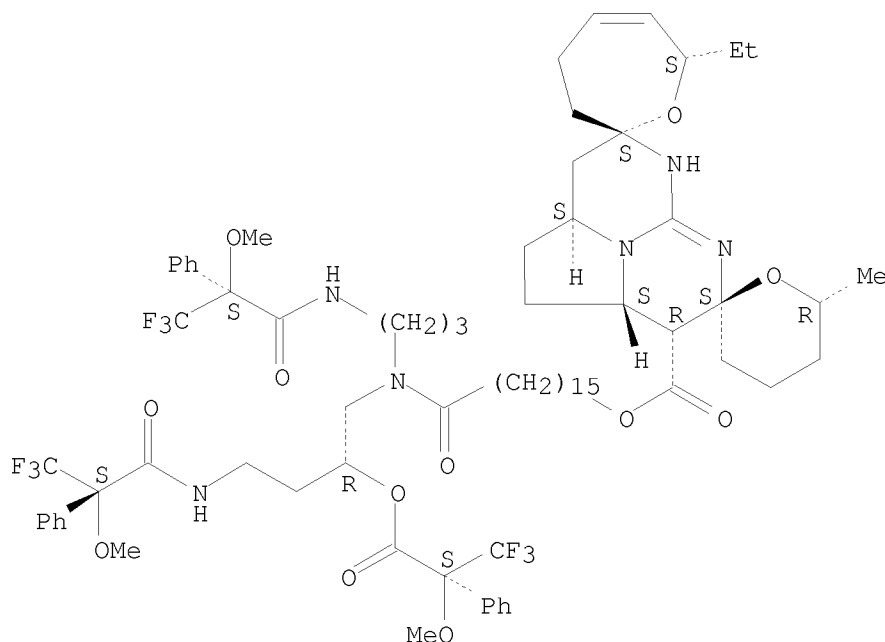


PAGE 2-A

● 3 HCl

RN 276878-03-6 CAPLUS
 CN Dispiro[oxepin-2(3H),4'-[4H-5,6,8b]triazacacenaphthylene-7'(5'H),2''-[2H]pyran]-8'-carboxylic acid, 7-ethyl-1',2',2'a,3',3'',4,4'',5'',6'',7,8',8'a-dodecahydro-6''-methyl-, 16-oxo-16-[[(2R)-2-[(2S)-3,3,3-trifluoro-2-methoxy-1-oxo-2-phenylpropoxy]-4-[[(2S)-3,3,3-trifluoro-2-methoxy-1-oxo-2-phenylpropyl]amino]butyl][3-[[(2S)-3,3,3-trifluoro-2-methoxy-1-oxo-2-phenylpropyl]amino]propyl]amino]hexadecyl ester, trihydrochloride, (2S,2''S,2'aS,6''R,7S,8'R,8'aS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



● 3 HCl

OS.CITING REF COUNT: 29 THERE ARE 29 CAPLUS RECORDS THAT CITE THIS
RECORD (29 CITINGS)
REFERENCE COUNT: 34 THERE ARE 34 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L19 ANSWER 4 OF 10 CAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 1999:803805 CAPLUS

DOCUMENT NUMBER: 132:222814

TITLE: Stereoselective synthesis of allylic amines by
rearrangement of allylic trifluoroacetimidates:
stereoselective synthesis of polyoxamic acid and
derivatives of other α -amino acids

AUTHOR(S): Savage, Ian; Thomas, Eric J.; Wilson, Peter D.

CORPORATE SOURCE: The Dyson Perrins Laboratory, Oxford, OX1 3QY, UK

SOURCE: Journal of the Chemical Society, Perkin Transactions
1: Organic and Bio-Organic Chemistry (1999), (22),
3291-3303

CODEN: JCPRB4; ISSN: 0300-922X

PUBLISHER: Royal Society of Chemistry

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 132:222814

AB On heating in xylene under reflux, allylic trifluoroacetimidates undergo
[3,3]sigmatropic rearrangement to regioisomeric allylic
trifluoroacetamides. Examples include the rearrangements of the
trifluoroacetimidates 16 and 73 to the trifluoroacetamides 17 and 74,
which were incorporated into stereoselective syntheses of polyoxamic acid
1, and the rearrangement of the trifluoroacetimide 26. The
rearrangement was the key step in asym. syntheses of the (S)- and

(R)-valine derivs. 37 and 48. Other examples include rearrangements of the trifluoroacetimidates 52, 54 and 56 prepared from geraniol, cinnamyl alc. and sorbyl alc., resp., and the more complex trifluoroacetimidates 62 and 69. The stereoselectivity of these rearrangements, which are somewhat faster than rearrangements of analogous allylic trichloroacetimidates, is consistent with the participation of chair-like, six-membered, transition structures.

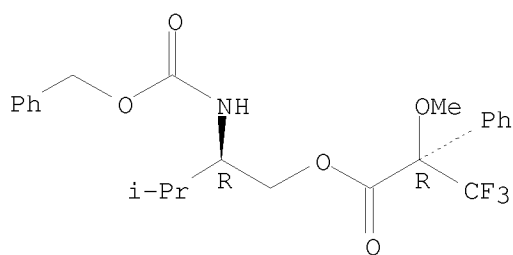
IT 260978-45-8P

RL: SPN (Synthetic preparation); PREP (Preparation)
(stereoselective synthesis of polyoxamic acid and derivs. of other α -amino acids by rearrangement of allylic trifluoroacetimidates)

RN 260978-45-8 CAPLUS

CN Benzeneacetic acid, α -methoxy- α -(trifluoromethyl)-,
(2R)-3-methyl-2-[[(phenylmethoxy)carbonyl]amino]butyl ester, (α R)-
(CA INDEX NAME)

Absolute stereochemistry.



OS.CITING REF COUNT: 28 THERE ARE 28 CAPLUS RECORDS THAT CITE THIS RECORD (28 CITINGS)

REFERENCE COUNT: 39 THERE ARE 39 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L19 ANSWER 5 OF 10 CAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 1998:323285 CAPLUS

DOCUMENT NUMBER: 129:16513

ORIGINAL REFERENCE NO.: 129:3549a,3552a

TITLE: Aqueous fluoropolymer compositions and their preparing methods

INVENTOR(S): Fan, Wei-qiang; Manzara, Anthony P.

PATENT ASSIGNEE(S): Minnesota Mining and Manufacturing Co., USA

SOURCE: PCT Int. Appl., 79 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9820055	A1	19980514	WO 1997-US4446	19970319
W:	AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GE, GH, HU, IL, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, TJ, TM, TR, TT, UA, UG, UZ, VN, YU			
RW:	GH, KE, LS, MW, SD, SZ, UG, AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG			
US 5998521	A	19991207	US 1996-743573	19961104
AU 9722184	A	19980529	AU 1997-22184	19970319
EP 935621	A1	19990818	EP 1997-915175	19970319
EP 935621	B1	20011128		

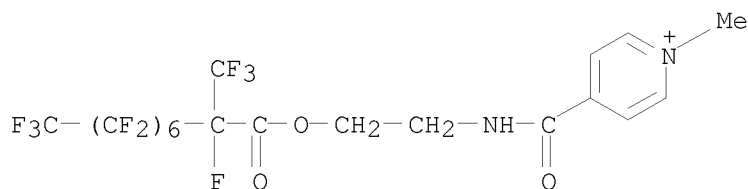
OTHER SOURCE(S) : MARPAT 129:16513

IT 207678-05-5P 207678-06-6P 207678-10-2P
207678-11-3P

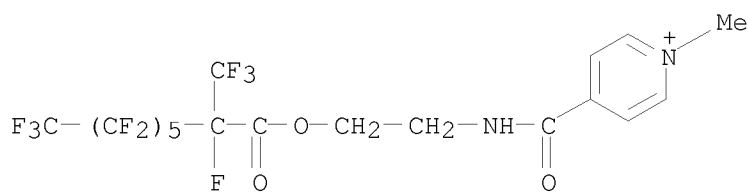
emulsifiers)

F3C(CF2)6C(F)(CF3)C(=O)OCCNC(=O)c1ccc(cc1)[N+]([O-])=OF3C(CF2)5C(F)(CF3)C(=O)OCCNC(=O)c1ccc(cc1)[N+]([O-])=O

CN Pyridinium, 4-[[[2-[[[2,3,3,4,4,5,5,6,6,7,7,8,8,9,9-hexadecafluoro-1-oxo-2-(trifluoromethyl)nonyl]oxy]ethyl]amino]carbonyl]-1-methyl-, iodide (1:1)
 (CA INDEX NAME)

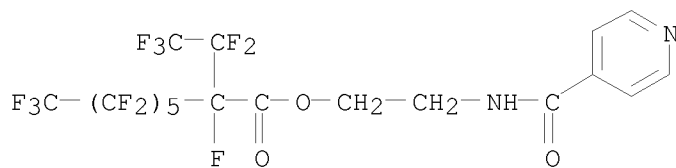


RN 207678-11-3 CAPLUS
 CN Pyridinium, 1-methyl-4-[[[2-[[2,3,3,4,4,5,5,6,6,7,7,8,8,8-tetradecafluoro-1-oxo-2-(trifluoromethyl)octyl]oxy]ethyl]amino]carbonyl]-, iodide (1:1)
 (CA INDEX NAME)

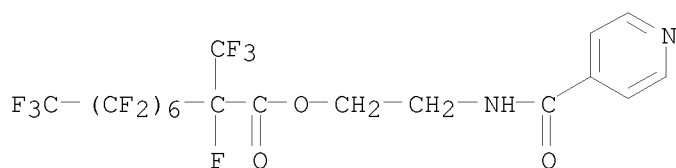


IT 207677-81-4P 207677-82-5P 207677-83-6P
 207677-84-7P
 RL: IMF (Industrial manufacture); RCT (Reactant); PREP (Preparation); RACT
 (Reactant or reagent)
 (aqueous fluoropolymer compns. containing environmentally-friendly
 fluorinated
 emulsifiers)

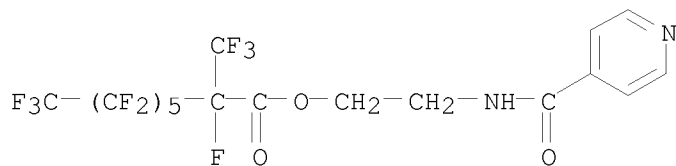
RN 207677-81-4 CAPLUS
 CN Octanoic acid, 2,3,3,4,4,5,5,6,6,7,7,8,8,8-tetradecafluoro-2-(1,1,2,2,2-pentafluoroethyl)-, 2-[(4-pyridinylcarbonyl)amino]ethyl ester (CA INDEX NAME)



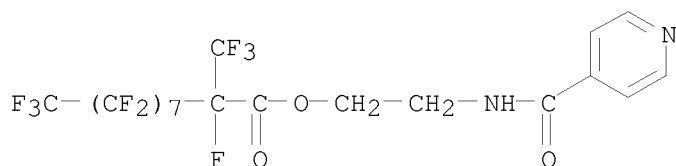
RN 207677-82-5 CAPLUS
 CN Nonanoic acid, 2,3,3,4,4,5,5,6,6,7,7,8,8,9,9,9-hexadecafluoro-2-(trifluoromethyl)-, 2-[(4-pyridinylcarbonyl)amino]ethyl ester (CA INDEX NAME)



RN 207677-83-6 CAPLUS
 CN Octanoic acid, 2,3,3,4,4,5,5,6,6,7,7,8,8,8-tetradecafluoro-2-(trifluoromethyl)-, 2-[(4-pyridinylcarbonyl)amino]ethyl ester (CA INDEX NAME)



RN 207677-84-7 CAPLUS
 CN Decanoic acid, 2,3,3,4,4,5,5,6,6,7,7,8,8,9,9,10,10,10-octadecafluoro-2-(trifluoromethyl)-, 2-[(4-pyridinylcarbonyl)amino]ethyl ester (CA INDEX NAME)



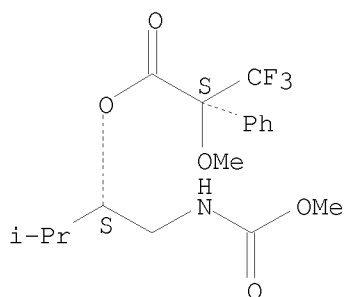
OS.CITING REF COUNT: 2 THERE ARE 2 CAPLUS RECORDS THAT CITE THIS RECORD (2 CITINGS)
 REFERENCE COUNT: 5 THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L19 ANSWER 6 OF 10 CAPLUS COPYRIGHT 2009 ACS on STN
 ACCESSION NUMBER: 1997:245213 CAPLUS
 DOCUMENT NUMBER: 126:330232
 ORIGINAL REFERENCE NO.: 126:64183a,64186a
 TITLE: A convenient method for synthesis of optically active β -hydroxyamines from primary amines through enecarbamates as key intermediates
 AUTHOR(S): Matsumura, Yoshihiro; Ohishi, Takahiro; Sonoda, Chihiro; Maki, Toshihide; Watanabe, Mitsuaki
 CORPORATE SOURCE: Fac. Pharmaceutical Sci., Nagasaki Univ., Nagasaki, 852, Japan
 SOURCE: Tetrahedron (1997), 53(13), 4579-4592
 CODEN: TETRAB; ISSN: 0040-4020
 PUBLISHER: Elsevier
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 OTHER SOURCE(S): CASREACT 126:330232
 AB This report describes a new method to prepare optically active β -hydroxyamines starting from primary amines. The method consists of a transformation of N-methoxycarbonylated primary amines to the corresponding enecarbamates utilizing electrochem. oxidation, and an asym. hydroboration of the enecarbamates to produce optically active

β -hydroxyamines.

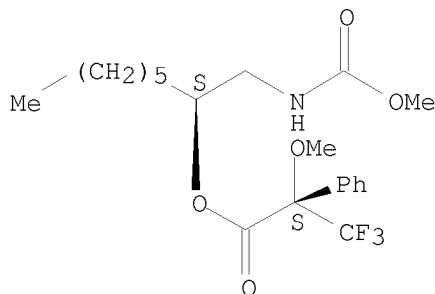
IT 189624-28-0P 189624-29-1P 189624-30-4P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of optically active β -hydroxy amines from primary amines
via enecarbamates)
RN 189624-28-0 CAPLUS
CN Benzeneacetic acid, α -methoxy- α -(trifluoromethyl)-,
1-[[(methoxycarbonyl)amino]methyl]-2-methylpropyl ester, [S-(R*,R*)]-
(9CI) (CA INDEX NAME)

Absolute stereochemistry.



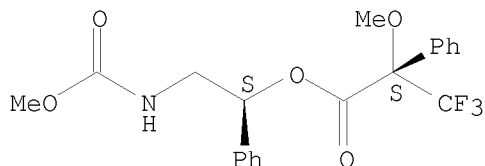
RN 189624-29-1 CAPLUS
CN Benzeneacetic acid, α -methoxy- α -(trifluoromethyl)-,
(1S)-1-[[(methoxycarbonyl)amino]methyl]heptyl ester, (α S)- (CA
INDEX NAME)

Absolute stereochemistry.



RN 189624-30-4 CAPLUS
CN Benzeneacetic acid, α -methoxy- α -(trifluoromethyl)-,
2-[(methoxycarbonyl)amino]-1-phenylethyl ester, [S-(R*,R*)]- (9CI) (CA
INDEX NAME)

Absolute stereochemistry.



OS.CITING REF COUNT: 7 THERE ARE 7 CAPLUS RECORDS THAT CITE THIS RECORD
(7 CITINGS)
REFERENCE COUNT: 38 THERE ARE 38 CITED REFERENCES AVAILABLE FOR THIS

L19 ANSWER 7 OF 10 CAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 1993:621081 CAPLUS

DOCUMENT NUMBER: 119:221081

ORIGINAL REFERENCE NO.: 119:39313a,39316a

TITLE: Identification and quantification of γ -glutamyl conjugates of biogenic amines in the nervous system of the snail, *Helix aspersa*, by gas chromatography-negative-ion chemical ionization mass spectrometry

AUTHOR(S): Zhou, P.; Watson, D. G.; Midgley, J. M.

CORPORATE SOURCE: Dep. Pharm. Sci., Univ. Strathclyde, Glasgow, G1 1XW, UK

SOURCE: Journal of Chromatography, Biomedical Applications (1993), 617(1), 11-18

CODEN: JCBADL; ISSN: 0378-4347

DOCUMENT TYPE: Journal

LANGUAGE: English

AB The γ -glutamyl conjugates of p-octapamine and dopamine were identified unambiguously for the first time and quantified in a single cerebral ganglion or pleural plus pedal ganglia of *Helix aspersa* by the title method. A new method was used for synthesis of γ -glutamylamine stds. The concentration of γ -glutamyltyramine was low in the tissues; therefore it was used as an internal standard. The γ -glutamylamines were extracted with water and derivatized with pentafluoropropionic anhydride and trifluoroethanol. Under neg.-ion chemical ionization conditions, the trifluoroethyl and pentafluoropropionyl derivs. produced significant ions which were sufficiently abundant to be suitable for selective ion monitoring. The method had a limit of detection of about 80 pg of γ -glutamyl conjugate per tissue and calibration curves were linear over the range examined

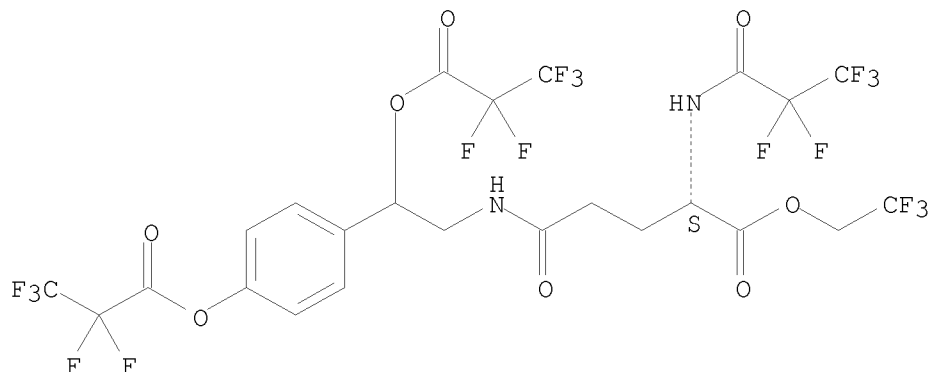
IT 150936-87-1 150936-89-3

RL: ANST (Analytical study)
(Kovats indexes and ion intensities of)

RN 150936-87-1 CAPLUS

CN L-Glutamine, N-[2-(2,2,3,3,3-pentafluoro-1-oxopropoxy)-2-[4-(2,2,3,3,3-pentafluoro-1-oxopropoxy)phenyl]ethyl]-N2-(2,2,3,3,3-pentafluoro-1-oxopropyl)-, 2,2,2-trifluoroethyl ester (CA INDEX NAME)

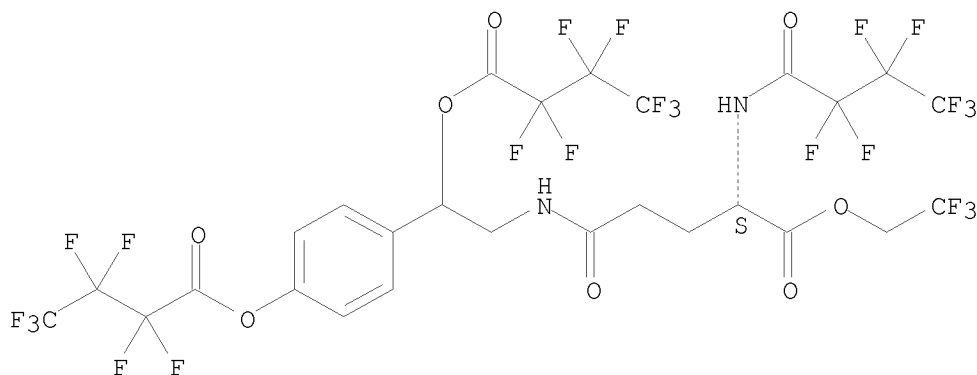
Absolute stereochemistry.



RN 150936-89-3 CAPLUS

CN L-Glutamine, N-[2-(2,2,3,3,4,4,4-heptafluoro-1-oxobutoxy)-2-[4-(2,2,3,3,4,4,4-heptafluoro-1-oxobutoxy)phenyl]ethyl]-N2-(2,2,3,3,4,4,4-heptafluoro-1-oxobutyl)-, 2,2,2-trifluoroethyl ester (CA INDEX NAME)

Absolute stereochemistry.



OS.CITING REF COUNT: 4 THERE ARE 4 CAPLUS RECORDS THAT CITE THIS RECORD
(4 CITINGS)

L19 ANSWER 8 OF 10 CAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 1984:468705 CAPLUS

DOCUMENT NUMBER: 101:68705

ORIGINAL REFERENCE NO.: 101:10559a,10562a

TITLE: A site specific rearrangement in electron capture negative ion CI mass spectrometry of pentafluoropropionyl derivatives of some β -hydroxyamines

AUTHOR(S): Low, G. K. C.; Duffield, A. M.

CORPORATE SOURCE: Biomed. Mass Spectrometry, Univ. New South Wales, Kensington, 2033, Australia

SOURCE: Biomedical Mass Spectrometry (1984), 11(4), 177-81
CODEN: BMSYAL; ISSN: 0306-042X

DOCUMENT TYPE: Journal

LANGUAGE: English

AB A rearrangement process observed in electron-capture neg.-ion chemical-ionization mass spectrometry of pentafluoropropionate (PFP) and heptafluorobutyrate (HFB) derivs. of some β -hydroxylated amines is reported. The pentafluoropropionate derivs. of a number of these substituted amines yield a prominent anion of mass 145 (195 in the corresponding heptafluorobutyrate derivs.). In the pentafluoropropionate derivs. of ethanolamine and β -hydroxyphenethylamine this anion was quant. displaced to m/z 146 when the γ -hydrogen (relative to the derivatized hydroxyl group) was substituted by deuterium. An initial 6-membered transition state was postulated to produce a pentafluoropropionic acid anion (not observed) which then eliminates either a H atom to give m/z 163 or a F atom to give m/z 145. The former remains at mass 163 in the γ -deuterated compds. examined. The proposed rearrangement is the neg. ion analog of the McLafferty rearrangement process of pos.-ion electron-impact mass spectrometry. However, the neg. ion rearrangement is not as general as its pos. ion electron impact counterpart because the former is critically dependent upon the substitution present on the α and β carbon and N atoms, resp., of the β -hydroxyamine-PFP (or HFB) derivs. In this regard, the effects on m/z 145 anion formation of Me substitution on the N and α and β C atoms of these pentafluoropropionate derivs. were examined. The results suggest that electron capture methane neg.-ion chemical-ionization mass spectra of β -hydroxylated PFP derivs. could be used as diagnostic tool for structural assignments within this group of compds.

IT 91224-21-4 91224-22-5 91224-25-8

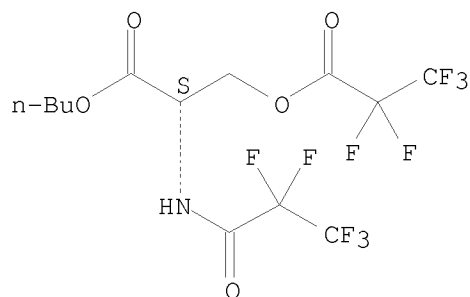
RL: PRP (Properties)

(mass spectrometry of, electron-capture neg.-ion chemical-ionization, site-specific rearrangement in)

RN 91224-21-4 CAPLUS

CN L-Serine, N-(2,2,3,3,3-pentafluoro-1-oxopropyl)-, butyl ester,
pentafluoropropanoate (ester) (9CI) (CA INDEX NAME)

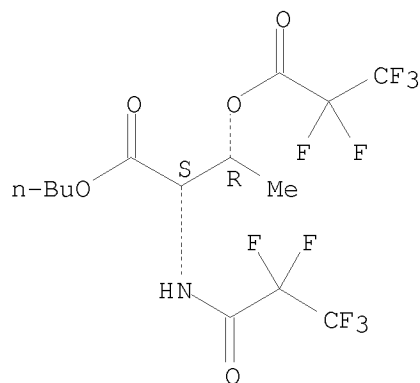
Absolute stereochemistry.



RN 91224-22-5 CAPLUS

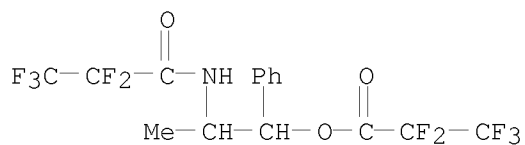
CN L-Threonine, N-(2,2,3,3,3-pentafluoro-1-oxopropyl)-, butyl ester,
pentafluoropropanoate (ester) (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 91224-25-8 CAPLUS

CN Propanoic acid, 2,2,3,3,3-pentafluoro-,
2-[(2,2,3,3,3-pentafluoro-1-oxopropyl)amino]-1-phenylpropyl ester (CA
INDEX NAME)



L19 ANSWER 9 OF 10 CAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 1984:451180 CAPLUS

DOCUMENT NUMBER: 101:51180

ORIGINAL REFERENCE NO.: 101:7907a,7910a

TITLE: Quantitative measurement of octopamines and
synephrines in urine using capillary column gas
chromatography negative ion chemical ionization mass
spectrometry

AUTHOR(S): Ibrahim, Kamal E.; Couch, Margaret W.; Williams, Clyde

M.; Budd, Mary Beth; Yost, Richard A.; Midgley, John M.
 CORPORATE SOURCE: Veterans Adm. Med. Cent., Univ. Florida, Gainesville, FL, 32610, USA
 SOURCE: Analytical Chemistry (1984), 56(9), 1695-9
 CODEN: ANCHAM; ISSN: 0003-2700
 DOCUMENT TYPE: Journal
 LANGUAGE: English

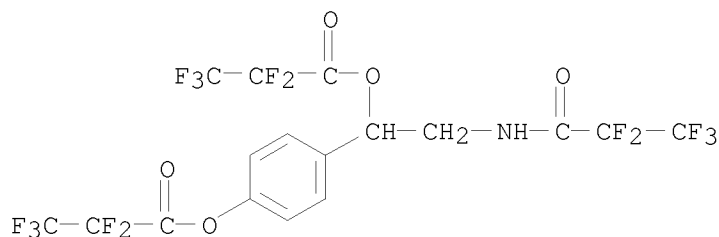
AB The isomeric octopamines and synephrines were measured in urine by assay which combines ion-exchange chromatog., capillary column gas chromatog., and electron-capture neg.-ion chemical-ionization mass spectrometry. Deuterium-labeled analogs of each compound were added to urine containing 1 mg creatinine and the acid hydrolyzate was subjected twice to cation-exchange chromatog. The resultant amine fraction was derivatized with pentafluoropropionic (PFP) anhydride and, under electron-capture neg. chemical ionization conditions, the PFP derivs. gave M- and (M - HF)- ions which were sufficiently abundant to be suitable for selected ion monitoring. The limit of detection was approx. 100 pg mg-1 creatinine. In normal adults, the concns. of o-, m-, and p-octopamine, and o-, m- and p-synephrine were, resp., 0.6, 2.1, 25, not detected 1.8, and 16 ng mg-1 creatinine. The occurrence of o- and m-octopamine and m-synephrine in human tissue or fluid has not been reported previously.

IT 62237-94-9 77745-52-9 90320-70-0
 90320-71-1 90320-72-2 90320-73-3

RL: PRP (Properties)
 (mass spectrum of)

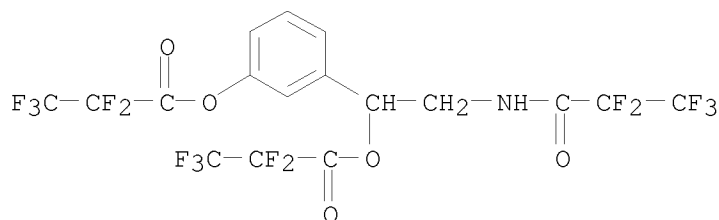
RN 62237-94-9 CAPLUS

CN Propanoic acid, pentafluoro-, 4-[1-(2,2,3,3,3-pentafluoro-1-oxopropoxy)-2-[(2,2,3,3,3-pentafluoro-1-oxopropyl)amino]ethyl]phenyl ester (9CI) (CA INDEX NAME)



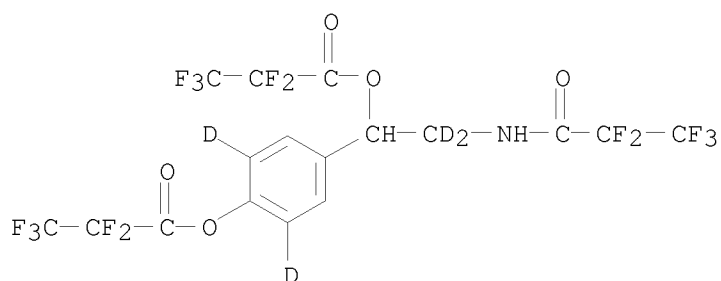
RN 77745-52-9 CAPLUS

CN Propanoic acid, pentafluoro-, 3-[1-(2,2,3,3,3-pentafluoro-1-oxopropoxy)-2-[(2,2,3,3,3-pentafluoro-1-oxopropyl)amino]ethyl]phenyl ester (9CI) (CA INDEX NAME)



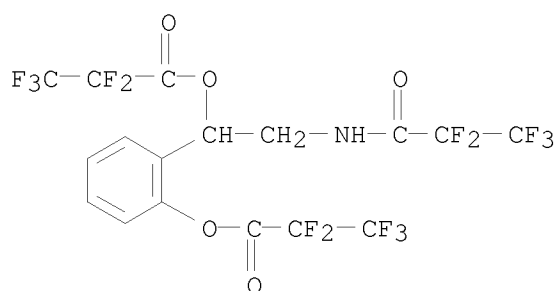
RN 90320-70-0 CAPLUS

CN Propanoic acid, pentafluoro-, 4-[1-(2,2,3,3,3-pentafluoro-1-oxopropoxy)-2-[(2,2,3,3,3-pentafluoro-1-oxopropyl)amino]ethyl-2,2-d2]phenyl-2,6-d2 ester (9CI) (CA INDEX NAME)



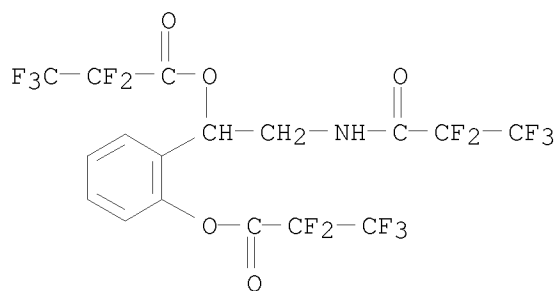
RN 90320-71-1 CAPLUS

CN Propanoic acid, pentafluoro-, 2-[1-(2,2,3,3,3-pentafluoro-1-oxopropoxy)-2-[(2,2,3,3,3-pentafluoro-1-oxopropyl)amino]ethyl]phenyl ester (9CI) (CA INDEX NAME)



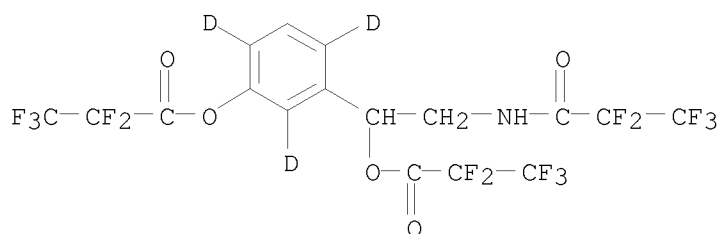
RN 90320-72-2 CAPLUS

CN Propanoic acid, pentafluoro-, 2-[1-(2,2,3,3,3-pentafluoro-1-oxopropoxy)-2-[(2,2,3,3,3-pentafluoro-1-oxopropyl)amino]ethyl]phenyl ester, labeled with deuterium (9CI) (CA INDEX NAME)



RN 90320-73-3 CAPLUS

CN Propanoic acid, pentafluoro-, 3-[1-(2,2,3,3,3-pentafluoro-1-oxopropoxy)-2-[(2,2,3,3,3-pentafluoro-1-oxopropyl)amino]ethyl]phenyl-2,4,6-d3 ester (9CI) (CA INDEX NAME)



OS.CITING REF COUNT: 9 THERE ARE 9 CAPLUS RECORDS THAT CITE THIS RECORD
(9 CITINGS)

L19 ANSWER 10 OF 10 CAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 1976:403011 CAPLUS

DOCUMENT NUMBER: 85:3011

ORIGINAL REFERENCE NO.: 85:491a,494a

TITLE: Studies in organic mass spectrometry. XV. Mass fragmentographic identification of epinine in adrenal medulla and as a product of an in vitro enzymic methylation

AUTHOR(S): Claeys, M.; Verzele, M.; Vandewalle, M.; Leysen, J.; Laduron, P.

CORPORATE SOURCE: Dep. Org. Chem., State Univ. Ghent, Ghent, Belg.

SOURCE: Biomedical Mass Spectrometry (1974), 1(2), 103-8

CODEN: BMSYAL; ISSN: 0306-042X

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Mass fragmentog. as the perfluoropropionate showed that epinine was present in pig adrenal medulla and in in vitro enzymic reaction mixts. using dopamine as the substrate, S-adenosylmethionine as the Me donor, and N-methyltransferase as the enzyme. The results support the model proposing epinine as the immediate precursor of adrenaline in adrenal medulla.

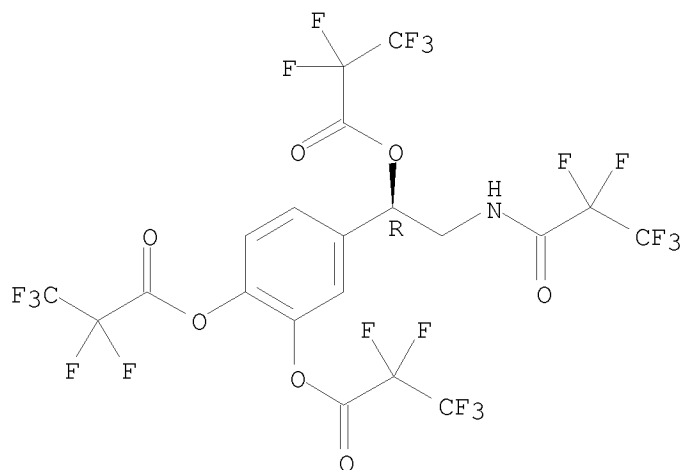
IT 55256-13-8

RL: PRP (Properties)
(mass spectrum of)

RN 55256-13-8 CAPLUS

CN Propanoic acid, pentafluoro-, 4-[1-(2,2,3,3,3-pentafluoro-1-oxopropoxy)-2-[(2,2,3,3,3-pentafluoro-1-oxopropyl)amino]ethyl]-1,2-phenylene ester, (R)-(9CI) (CA INDEX NAME)

Absolute stereochemistry.



=> s isocyanate

L24 73699 ISOCYANATE

=> s 124 and triethylamine

38935 TRIETHYLAMINE

L25 1022 L24 AND TRIETHYLAMINE

=> s 125 and acrylate

212923 ACRYLATE
L26 125 L25 AND ACRYLATE

=> s 126 and chloro
373397 CHLORO
L27 8 L26 AND CHLORO

=> d 127 ibib abs 1-
YOU HAVE REQUESTED DATA FROM 8 ANSWERS - CONTINUE? Y/(N):y

L27 ANSWER 1 OF 8 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 2009:435012 CAPLUS
DOCUMENT NUMBER: 150:521387
TITLE: Prediction of the Upper Flammability Limits of Organic Compounds from Molecular Structures
AUTHOR(S): Pan, Yong; Jiang, Juncheng; Wang, Rui; Cao, Hongyin; Cui, Yi
CORPORATE SOURCE: Jiangsu Key Laboratory of Urban and Industrial Safety, Institute of Safety Engineering, Nanjing University of Technology, Nanjing, 210009, Peop. Rep. China
SOURCE: Industrial & Engineering Chemistry Research (2009), 48(10), 5064-5069
CODEN: IECRED; ISSN: 0888-5885
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English

AB A quant. structure-property relationship (QSPR) study was performed to develop math. models to predict upper flammability limits (UFL) for organic compds. from their mol. structures. Organic compound structural features were numerically represented by various types of calculated mol. descriptors (e.g., topol., charge, geometric). A genetic algorithm combined with multiple linear regression (GA-MLR) was used to select an optimal descriptor subset which significantly contributed to overall UFL from the large pool of calculated descriptors. The best resulted model was a 4-variable, multi-linear model with a defined applicability range. Average absolute and root-mean-square errors obtained from an external test set were 1.75 volume percent and 2.77, resp. The proposed model can predict organic compound UFL using only 4 pre-selected theor. descriptors which can be directly calculated from mol. structure alone.

REFERENCE COUNT: 32 THERE ARE 32 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L27 ANSWER 2 OF 8 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 2006:410748 CAPLUS
DOCUMENT NUMBER: 146:1771
TITLE: Quantitative structure-activity relationship models for prediction of sensory irritants (logRD50) of volatile organic chemicals
AUTHOR(S): Luan, Feng; Ma, Weiping; Zhang, Xiaoyun; Zhang, Haixia; Liu, Mancan; Hu, Zhide; Fan, B. T.
CORPORATE SOURCE: Department of Chemistry, Lanzhou University, Lanzhou, 730000, Peop. Rep. China
SOURCE: Chemosphere (2006), 63(7), 1142-1153
CODEN: CSMHAF; ISSN: 0045-6535
PUBLISHER: Elsevier B.V.
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Quant. classification and regression models for prediction of sensory irritants (log RD50) of volatile organic chems. (VOCs) have been developed. Each compound was represented by the calculated structural descriptors to encode constitutional, topol., geometrical, electrostatic, and quantum-chemical features. The heuristic method (HM) was then used to search the

descriptor space and select the descriptors responsible for activity. The best classification results were found using support vector machine (SVM): the accuracy for training, test and overall data set is 96.5%, 85.7% and 94.4%, resp. The nonlinear regression models were built by radial basis function neural networks (RNFNN) and SVM, resp. The root mean squared errors (RMS) in prediction for the training, test and overall data set are 0.4755, 0.6322 and 0.5009 for reactive group, 0.2430, 0.4798 and 0.3064 for nonreactive group by RBFNN. The comparative results obtained by SVM are 0.4415, 0.7430 and 0.5140 for reactive group, 0.3920, 0.4520 and 0.4050 for nonreactive group, resp. This paper proposes an effective method for poisonous chems. screening and considering.

OS.CITING REF COUNT: 8 THERE ARE 8 CAPLUS RECORDS THAT CITE THIS RECORD (8 CITINGS)
REFERENCE COUNT: 39 THERE ARE 39 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L27 ANSWER 3 OF 8 CAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 2000:96012 CAPLUS
DOCUMENT NUMBER: 132:137818
TITLE: Production of macromonomer with two or more polycondensable equally reactive functional groups from carboxyl- or hydroxyl-containing prepolymer
INVENTOR(S): Ramanathan, Lalgudi Srinivasan; Sivaram, Swaminathan
PATENT ASSIGNEE(S): Council of Scientific & Industrial Research, India
SOURCE: U.S., 5 pp.
CODEN: USXXAM
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 6022930	A	20000208	US 1998-143028	19980828
IN 1998DE01635	A	20050909	IN 1998-DE1635	19980612
PRIORITY APPLN. INFO.:			IN 1998-DE1635	A 19980612

AB A process for producing a title macromonomer -R1[C(COOR)CH2]nXR2C(O)OC(F)m, where R is C1-40 alkyl; R1 is H or Me; R2 is alkylene; X is bifunctional moiety; F is a functional group; n = 3-45; and m ≥ 2, comprises (a) preparing a carboxyl- or hydroxyl-terminated prepolymer by polymerizing a monomer such as Me methacrylate in the presence of a bifunctional agent such as mercaptoacetic acid or 2-mercaptoethanol; (b) reacting the prepolymer with an organic compound containing two or more isocyanate reactive functional groups in the presence of a dehydrating agent such as dicyclohexylcarbodiimide and a nonreactive organic solvent; and (c) separating the product from the reaction mixture The prepolymer can be esterified directly with a multifunctional organic compound such as trimethylolpropane. The macromonomers may be useful in the production of tailored graft copolymers and as surface active agents, compatibilizers, adhesion promoters, organic coatings and biopolymers (no data).

OS.CITING REF COUNT: 2 THERE ARE 2 CAPLUS RECORDS THAT CITE THIS RECORD (2 CITINGS)
REFERENCE COUNT: 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L27 ANSWER 4 OF 8 CAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 1997:676378 CAPLUS
DOCUMENT NUMBER: 127:335828
ORIGINAL REFERENCE NO.: 127:65883a, 65886a
TITLE: Wood furniture manufacturing operations, NESHP implementation document
AUTHOR(S): Rasor, Susan A.

CORPORATE SOURCE: Midwest Research Institute, Cary, NC, 27511, USA
SOURCE: United States Environmental Protection Agency, Office
of Air Quality Planning and Standards, [Technical
Report] EPA (1997), EPA-456/R-97-005, 1-114
CODEN: UEPEDY
DOCUMENT TYPE: Report
LANGUAGE: English
AB National emissions stds. to control emissions of Hazardous Air Pollutants
(HAP) from new and existing wood furniture manufacturing operations were
promulgated in 1995. This document contains information to assist State
and local air pollution control agencies as well as the regulated
community in the implementation of these stds. This document provides a
common sense summary of the National Emission Stds. (NES) HAP requirements
and provides answers to commonly asked questions on the NESHAP. Sample
inspection sheets are also provided as is a bibliog. of Federal, State and
private sources of addnl. information related to these stds.

L27 ANSWER 5 OF 8 CAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 1993:65829 CAPLUS
DOCUMENT NUMBER: 118:65829
ORIGINAL REFERENCE NO.: 118:11581a,11584a
TITLE: Air contaminants
CORPORATE SOURCE: Occupational Safety and Health Administration, U. S.
Dep. Labor, Washington, DC, 20210, USA
SOURCE: Federal Register (1992), 57(114, Bk. 2), 26002-601, 12
Jun 1992
CODEN: FEREAC; ISSN: 0097-6326
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Proposed amendments of existing air contaminant stds. for the maritime and
construction industries and extension of air contaminant stds. to
agricultural employees (only employees of farms with >10 nonfamily
employees are covered) are given under the Federal Occupational Safety and
Health Administration. Tables that indicated transitional limits, based
on established threshold limit values, indication of skin protection
needs, proposed time-weighted average exposure (any 8-h work shift for 40-h
week), short-term exposure limit (15-min time-weighted average), ceiling
(exposure during any part of the work day, or if instantaneous monitoring
is not feasible, the 15-min time-weighted average), and/or skin protection
needs are given for the shipyard, marine terminal and longshoring,
construction, and agricultural industries. Extensive data on health
effects of the substances to be regulated and preliminary regulatory
impact analyses are given for general industry and the specific industrial
sectors.

OS.CITING REF COUNT: 1 THERE ARE 1 CAPLUS RECORDS THAT CITE THIS RECORD
(1 CITINGS)

L27 ANSWER 6 OF 8 CAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 1992:135528 CAPLUS
DOCUMENT NUMBER: 116:135528
ORIGINAL REFERENCE NO.: 116:22789a,22792a
TITLE: Performance-oriented packaging standards; changes to
classification, hazard communication, packaging and
handling requirements based on UN standards and agency
initiative
CORPORATE SOURCE: United States Dept. of Transportation, Washington, DC,
20590-0001, USA
SOURCE: Federal Register (1990), 55(246), 52402-729, 21 Dec
1990
CODEN: FEREAC; ISSN: 0097-6326
DOCUMENT TYPE: Journal
LANGUAGE: English

AB The hazardous materials regulations under the Federal Hazardous Materials

Transportation Act are revised based on the United Nations recommendations on the transport of dangerous goods. The regulations cover the classification of materials, packaging requirements, and package marking, labeling, and shipping documentation, as well as transportation modes and handling, and incident reporting. Performance-oriented stds. are adopted for packaging for bulk and nonbulk transportation, and SI units of measurement generally replace US customary units. Hazardous material descriptions and proper shipping names are tabulated together with hazard class, identification nos., packing group, label required, special provisions, packaging authorizations, quantity limitations, and vessel stowage requirements.

L27 ANSWER 7 OF 8 CAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 1989:218230 CAPLUS
DOCUMENT NUMBER: 110:218230
ORIGINAL REFERENCE NO.: 110:36135a,36138a
TITLE: Air contaminants
CORPORATE SOURCE: United States Occupational Safety and Health
Administration, Washington, DC, 20210, USA
SOURCE: Federal Register (1989), 54(12, Bk. 2), 2332-983, 19
Jan 1989
CODEN: FEREAC; ISSN: 0097-6326
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Under the Federal Occupational Safety and Health act, OSHA is amending existing air containment stds. and setting new permissible exposure limits for toxic substances commonly used in the workplace.

L27 ANSWER 8 OF 8 CAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 1966:104956 CAPLUS
DOCUMENT NUMBER: 64:104956
ORIGINAL REFERENCE NO.: 64:19826a-h,19827a-d
TITLE: Thiocarbonyl fluorides and their polymers
INVENTOR(S): Middleton, William J.
PATENT ASSIGNEE(S): E. I. du Pont de Nemours & Co.
SOURCE: 8 pp.; Continuation in part of U.S. 2,980,695 (see
Brit. 857,649, CA 55, 11918g)
DOCUMENT TYPE: Patent
LANGUAGE: Unavailable
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
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US 3240765		19660315	US 1961-106533	19590604
PRIORITY APPLN. INFO.:			US	19590604

AB Addition homopolymers having a mol. weight of ≥ 2000 and with the repeating-SCFX-units are described, in which CSF₂ is especially suitable as the monomer. Heteropolymers are prepared by using CSFX and a thioacyl fluoride. Other hetero polymers are also prepared by using CSFX and a polymerizable unsatd. organic compound All of the homo- and heteropolymers exist as self-supporting structures. The polymers are preferably prepared at 0 to -120° in a solvent containing 0.2-20% HCONMe₂ for 1 h. to 4 days. CSF₂ was prepared from purified tetrafluoro-1,3-dithietane (b. 49°, m. 6°, n_{25D} x1.3908, d₂₀ 1.6036) by adding it dropwise during 2 h. at the top of a Pt tube, 0.5 in. in diameter and 25 in. long, inclined at an angle of 30°, and heated to 500° over a length of 12 in. A slow stream of He was passed through the tube during the pyrolysis. The exit gases were condensed in successive traps cooled by a mixture of acetone and dry ice and liquid N, resp. The combined materials from the traps were distilled through a 16-in. column packed with glass helixes. Thus, 34 g. of a colored liquid, b. -54°, was obtained. It was 98% pure. Thiocarbonyl chloride fluoride (I) was similarly prepared at 500° in

1 h. by using chlorotrifluoro-1,3-dithietane. Thus, 4.3 g. of a nearly colorless liquid CSF₂, b. -54°, was obtained along with 1.18 g. yellow I, b. 6°, and 1.38 g. red thiophosgene, b. 72-4°. Some CSF₂ (95.5% pure) was stored in a stainless-steel container for 6 wk at room temperature. A clear, sirupy residue, polythiocarbonyl fluoride (II), was obtained. It solidified to a white wax, m. 30-5°, when stored for 2 days in a vacuum desiccator. The mol. weight was 2150 as determined by

the

lowering of the f.p. in tetrachlorodifluoroethane. Freshly prepared CSF₂ from 20 g. of the dithietane) was transferred under N to a 100-cc. flask cooled to -80° and connected to a condenser cooled with dry ice.

As the liquid monomer was stirred, 1 cc. of a saturated solution of NaCN in HCONMe₂

was introduced rapidly through a syringe. The mixture began to solidify almost immediately. After 2 h. at -80°, a solid cake formed. As the cake was warmed to room temperature, the top layer became black and gummy. The cake was broken into pieces, removed from the flask, and the black portion separated. The white solid weighed 3.1 g. after washing with H₂O and drying. A film was pressed at 180° and 10,000 psi. for 15 s. The film was white and rubbery. It lost its rubbery character and became soft at 230° and decomposed into gaseous products at 270°. The film was still flexible, although somewhat stiffer when cooled to -80°. The black, gummy material was boiled with concentrated HNO₃ for 30 min. Most of the color was removed and 9.7 g. of a light-yellow II was obtained. It was also pressed to form a rubbery film. CSF₂ (1.5 g.) was also polymerized in tetrafluoro-1,3-dithietane at 75° for 3 h., 80° for 6 h., and 85° for 3 h. at 3000 atmospheric to give 1.2 g. white, waxy II, m. 35-40°. Some II prepared in C₅H₁₂ containing HCONMe₂ and NaCN at -80° for 2 h. gave a rubbery film when pressed at 150° and 10,000 psi. It had a zero-strength temperature of 231°. By using Et₂O in place of the C₅H₁₂ and polymerizing at -80° for 20 h., a white tough spongy polymer was obtained with an intrinsic viscosity of 3.7 (0.1% in CHCl₃ at 25°). A rubbery film was obtained by pressing at 150° and 12,000 psi. for 10 min. Under tension, the film was extended to 3 times its original length. The drawn film had a tensile strength of 10,800 psi. at 58% elongation. The polymer crystallized slowly at room temperature to a white, opaque, waxy plastic. When held at 36° (the m.p.), it reverted to an amorphous plastic form. A 2.23 in. ball of the II (molded at 150° and 6000 psi.) rebounded 90% of the distance from which it had been dropped. Copolymers were also prepared by using trifluorothioacetyl fluoride (III). A mixture of 20 cc. anhydrous Et₂O, 10.5 g. CSF₂ and 3 g. III was placed in a polymerization vessel cooled

with

acetone and dry ice and blanketed with He and a solution of 0.1 g. N-methylmorpholine in 5 cc. anhydrous Et₂O was added. After 5 h., a solid polymer had formed and the resulting mixture was poured into hot 1:1 HCl. The polymer was washed with H₂O and with Me₂CO and dried in a vacuum at 60°. The crude polymer (9.7 g.) was dissolved in 400 cc. of CHCl₃ and precipitated by addition of 50 cc. MeOH. The filtered and dried polymer

weighed

8.8 g. It was pressed to a limp, opaque film at 150° and 10,000 psi. The polymer slowly crystallized at room temperature. Its inherent viscosity was

1.19 (0.1% in CHCl₃ at 25°). Copolymers were also prepared from chlorofluorothioacetyl fluoride and CSF₂, perfluorocyclobutane and CSF₂. The resins prepared from CSF₂ or I with comonomers having CO₂H groups or groups readily converted to CO₂H groups can be cured with diepoxide compds. or comm. epoxy resins. For example, a copolymer of CSF₂ and Et acrylate was prepared from 20 parts of the former and 1 part of the latter in hexane at -80° using Et₃B and O as the catalyst. One part of this polymer was stirred at room temperature with 3.54 parts concentrated HCl in 44.4 parts THF for 4 days. The polymer was precipitated with H₂O and dried.

The polymer was well mixed with 0.04 part of Epon 1031 on a press at 75° by several pressings. The resultant mixture was then cured at 135° for 1 h. at 1000 psi. This cured polymer was no longer soluble in CHCl₃. One part of a copolymer of CSF₂ and tert-Bu acrylate containing 95.6 weight-% CSF₂ was mixed with 0.05 part Epotuf ED-1025 in 425 parts CHCl₃ and allowed to stand at room temperature for 20 h. The uniform gel which formed was pressed into a sheet at 50° to remove the CHCl₃. One portion of the sheet was cured at 140° for 3 h. under 2000 psi. The other portion was cured under the same conditions for 18 h. The material from the first pressing had an equilibrium gain in CHCl₃ of 250%. The material from the second pressing had an equilibrium weight gain of 100%. The uncured composition was completely soluble in CHCl₃. The copolymers can also

be

vulcanized by using an unsatd. comonomer containing isocyanate, isothiocyanate, chloroformate, or acyl halide groups by reaction with a reagent containing at least 2 reactive H atoms attached to an O or N atom, e.g. an amide, an amine, NH₃, alc., or H₂O. For example, 100 parts of a copolymer containing 95% CSF₂ and 5% allyl chloroformate was mixed with 3 parts sym.-diisopropylurea on a press at 50° and cured at 100° with 1000 psi. for 1 h. The cured polymer was no longer soluble in CHCl₃ and had improved tensile properties at elevated temps. Also, 1 part of a copolymer of CSF₂ and α,α -dimethallyl isocyanate was mixed with 0.05 part methylene bis(o-chloroaniline) by pressing at 100°. It was then cured at 100° for 1 h. at 10,000 psi. The cured polymer did not flow at elevated temps. under stress and was insol. in CHCl₃. In addition to having a high degree of

chemical

inertness, they are soluble in some organic solvents and may be used as coatings. They are especially useful for making fabrics water repellent.

Thus,

a 2% solution of a polymer containing 86% CSF₂ and 14% α,α -dimethallyl isocyanate in xylene was prepared. Swatches of cotton, cellulose acetate, Dacron, nylon and Orlon fabrics were immersed in the above solution for 3 h. at 150°, and air dried. Drops of H₂O were not absorbed by the fabrics in 15 min. The swatches were still water repellent after 3 launderings and 3 dry cleanings with perchloroethylene. They were still water repellent after a final washing at 90-95°, and air drying. The high-mol. weight polymers have m.ps. which permit them to be shaped by extrusion, by molding, or by pressing.